



A Bond-Order Potential for Atomistic Simulations in Iron

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Abstract

A new semi-empirical potential in iron (Fe) has been developed based on the quantum chemistry concept of bond order. The new potential was calibrated using the traditional fitting to the universal scaling and the equilibrium volume and cohesive energy of base-centered cubic (BCC) iron. With a total of 15 fitted parameters, the potential reproduces with only minor deviations to the elastic moduli, the volume-pressure equation of states in the BCC phase, the energies in face-centered cubic (FCC) and hexagonal close packing (HCP) modifications, the BCC-HCP phase transformation under pressure, and the energy of the (111) free surface.

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1. Introduction

Among the elemental solids which have received special attention in materials theory and applications, iron (Fe) is rather unique in its scientific and technological importance. These areas of importance range from an understanding of the earth's inner core in seismology, to structural applications such as radiation embrittlement of nuclear reactor pressure vessels (Wirth et al. 1997) and toughness of high-strength iron-based alloys. In fact, in spite of emerging families of new nonmetallic materials, iron still constitutes the technological core of our civilization.

After decades of research on iron and steel, a renewed comprehensive attack on this material may not appear particularly timely until one realizes that the fundamental understanding of many important properties (such as deformation and plasticity of base-centered cubic [BCC] transition metals or chemisorption of gases at free surfaces) still does not exist. In crystalline solids, the mechanisms which govern the bifurcation of behavior between brittle and ductile responses, as well as the processes at free surfaces, reside fundamentally at the atomic level.

Ever since the early days of computational modeling, developing the capability to reliably predict the strength and other physical properties of iron has been a recognized challenge. In the current context of modeling the properties and behaviors of materials across various length scales, there continues to be interest in gaining a more fundamental and quantitative understanding of how iron deforms under stress and behaves under other physical or chemical exposures.

Two approaches currently exist for modeling iron. Development in the recent decade of efficient methods of *ab-initio* calculations and proliferation of high-speed computers made it possible to perform high-precision first-principles calculations on iron. This approach has essentially improved our understanding of structural properties of iron under high pressure (Soderling et al. 1996), as well as elucidated the energetics of important polymorphic transformations in iron: BCC face-centered cubic (FCC) (Krasko 1987, 1989; Krasko and Olson 1989) and BCC-hardness critical process (HCP) (Eckman et al. 1998; Sob et al., to be published).

Ab-initio modeling of iron grain boundaries has resulted in an understanding, on atom-electron level, of the effect of interstitial impurities on cohesion-decohesion processes at grain boundaries and of grain-boundary embrittlement (Krasko and Olson 1990; Wu et al. 1994a, 1994b, 1996). The state-of-the-art *ab-initio* calculations on iron-free surfaces has enabled one to better understand the multilayer relaxation and chemisorption of hydrogen (Wu and Freeman 1993a, 1993b; Krasko et al., to be published).

However, the *ab-initio* approach at the present time has two fundamental limitations. Firstly, it cannot be used for high temperature studies; secondly, modeling processes involving atomistically large systems (even of a few hundred atoms) are still outside of our computational capacity. As an alternative, certain aspects of physical behavior can be simulated at the atomistic level, where interatomic interactions are described by empirical (or semi-empirical) potential models. However, the physical rigor of such results may be uncertain or suspect due to inadequacy of the potential description.

In atomistic simulations, often one has to strike a balance between the robustness and accuracy of the model and the computational feasibility of the study. BCC transition metals pose particular challenges because the validity of using empirical classical potential functions is well known as questionable. On the one hand, properties such as strong directional bonding and ferromagnetism make it necessary to explicitly consider the electronic degrees of freedom in describing the interatomic interactions.

Practically all current atomistic simulations in iron are concerned with BCC structure using variants of a many-body potential in one of two forms: the so-called embedded atom method (EAM) (Baskes et al. 1988; Daw and Baskes 1984; Foils et al. 1986; Daw 1989), and the so-called N-body or Finnis-Sinclair (FS) potential (Finnis and Sinclair 1984, 1986).

The EAM (Baskes et al. 1988; Daw and Baskes 1984; Foils et al. 1986; Daw 1989)—the method of choice in virtually all atomistic simulations—is based on the concept of substituting a uniform “embedding” jelly for a real atomic environment. This idea originates from the so called

“effective medium” theory, but has been made much more robust by incorporating experimental information for fitting the model parameters.

According to EAM, the total energy of a condensed-matter system can be written as

$$E = \sum_i F[\rho(R_i)] + 1/2 \sum_{i,j} V_{\text{rep}}(|R_i - R_j|), \quad (1)$$

where $F[\rho(R)]$ is the “embedding function,” $\rho(R)$ is a quantity characterizing the local atomic environment (e.g., the free atom electron charge density at the atomic site R due to the surrounding atoms), and $V_{\text{rep}}(R_i - R_j)$ is a repulsive pair potential. In the original EAM, both F and V were model functions that depended on a number of parameters being fit to a set of experimental data; this typically includes the cohesive energy in the system at equilibrium, the equilibrium lattice parameter, the elastic moduli, and possibly the energies of metastable configurations such as the vacancy formation energy.

Although the nature and shape of the pair potential is rather clear, the electrostatic repulsion (the functional form of the embedding function) may only be guessed. Quite a few different forms of F and other ideas have been suggested since the EAM was formulated; these models are sometimes referred to as “glue models” (Heine and Hafner 1990).

As mentioned previously, a vast family of EAM-type models for iron have been developed thus far (Simonelly et al. 1995). The most advanced models, allowing for directionality of interatomic bonds, actually explore two ideas: (1) the tight-binding analysis utilizing moments of the electronic density of states (Carlsson 1991) and (2) the well-known concept of bond order (BO) from quantum chemistry (Horsfield 1996; Horsfield et al. 1996; Aoki et al. 1997; Abel 1985). In recent years, the BO-type empirical potentials have been widely used in atomistic modeling of diamond-structure semiconductors and their alloys and compounds (Tersoff 1988a, 1988b, 1988c, 1989; Tang and Yip 1995a, 1995b).

The environmental parameter in the so-called modified embedded atom method (MEAM) (Baskes 1997), still interpreted as an electron density, has a nonspherical symmetry, which allows for directionality of bonds. In all the existing EAM-type models, both the pair potentials and the embedding functions are of a more or less arbitrary character, although in the founding papers (Daw and Baskes 1984; Foils et al. 1986; Daw 1989) the physical connection between the embedding function and the exchange-correlation energy of the density functional theory has been established.

Recently, a new approach explicitly allowing for ferromagnetic effects via the Stoner model has been suggested (Krasko 1996; Shibutani et al., to be published). In this report, however, we explore the ideas behind the Tersoff BO approach (Tersoff 1988a, 1988b, 1988c, 1989) and develop a BO potential to be used in atomistic simulations in iron.

Section 2 briefly outlines the BO concept and the Tersoff potential (Tersoff 1988a, 1988b, 1988c, 1989), which served as a prototype for our new potential. In section 3, we describe this potential and the procedure of fitting its parameters. Section 4 is a conclusion.

2. Bond-Order Concept and the Tersoff Potential

The BO concept follows directly from quantum chemistry. Without going into much detail, we will briefly outline the origin of the BO term in the expression for the cohesive energy (one can find a concise discussion of the concept in Horsfield [1996]; Horsfield et al. [1996]; Aoki et al. [1997]; and Abel [1985]).

From the tight-binding or linear combination atomic orbital (LCAO) approach, the self-consistent-field Hamiltonian is written as (Abel 1985)

$$H = T + \sum_i V_i, \quad (2)$$

where T is the kinetic energy operator and V_i is the effective potential acting on atom i . It is believed to be short ranged and strongly localized. The summation in equation 2 is extended over all atoms. From here, an expression for a chemical pseudopotential immediately follows, with the Schrödinger equation

$$\{T + V_i + \sum_j (V_j - |\phi_j\rangle\langle\phi_j|V_j)\}|\phi_i\rangle = \epsilon_i|\phi_i\rangle. \quad (3)$$

Here, ϕ_i 's are the atomic-like local orbitals, and V_i is the self-consistent one-electron potential that includes both the electrostatic and exchange-correlation parts.

From this starting point, the expression for the cohesive energy is

$$E = \sum_i \{q_i \sum_{j \neq i} V_{\text{rep}}(R_{ij}) + \sum_{j \neq i} b_{ij} V_{\text{attr}}(R_{ij})\} \quad (4)$$

where $V_{\text{rep}}(R_{ij})$ is the repulsive and $V_{\text{attr}}(R_{ij})$ is the attractive interatomic potential between atoms i and j separated by distance R_{ij} . These potentials, in turn, are defined as

$$V_{\text{rep}}(R_{ij}) = \langle \phi_j^0 | V_i | \phi_j^0 \rangle - \langle \phi_i^0 | \phi_j^0 \rangle \langle \phi_i^0 | V_i | \phi_j^0 \rangle, \text{ and} \quad (5a)$$

$$V_{\text{attr}}(R_{ij}) = \langle \phi_i^0 | V_i | \phi_j^0 \rangle, \quad (5b)$$

where ϕ_i^0 's are the "unperturbed" atomic basis orbitals. Factor q_i is the electron charge density on atom i , while b_{ij} is the BO. The BO is the strength of the corresponding (ij) bond.

BO strongly depends on environment. The number of neighbors, Z , is the simplest environmental parameter. It was shown in Abel (1985) that at large Z is

$$b_{ij} \sim 1/\sqrt{Z}. \quad (6)$$

Having summed over the nearest neighbors, j , equation 4 will result in the attraction term proportional to \sqrt{Z} , which is exactly what the FS model (Finnis and Sinclair 1984, 1986) postulates. Equation 4, however, does not have a “glue” form.

In Abel (1985), the quantities entering equation 4 were parametrized by simple functions. In the recent decade, quite a few expressions for the both environmental parameter and the BO function were suggested (Balamante et al. 1992).

Among these models, the so-called Tersoff potentials (Tersoff 1988a, 1988b, 1988c, 1989) are of prime interest for our purposes. Formulated initially for silicon crystals, the potentials were also used for carbon and germanium, and later generalized to allow for multicomponent systems description (Tersoff 1988a, 1988b, 1988c, 1989; Tang and Yip 1995a, 1995b). The Tersoff potentials explicitly take into account the directionality of bonds. For a one-component covalent crystal, the total energy is taken to be

$$E = 1/2 \sum_i \sum_j f_c(R_i - R_j) [V_{rep}(R_i - R_j) + V_{bo}(R_i, R_j)] . \quad (7)$$

Here, $f_c(R)$ is the cut-off function, where

$$f_c(R) = \begin{cases} 1, & R < r_{c1} \\ 1/2 + 1/2 \cos [\pi(R - r_{c1})/(r_{c2} - r_{c1})], & r_{c1} \leq R < r_{c2}, \text{ and} \\ 0, & R > r_{c2} \end{cases} \quad (8)$$

r_{c1} and r_{c2} are the cut-off radii. The repulsive pair-wise potential, $V_{rep}(R_i - R)$, has the simple exponential form

$$V_{rep}(R) = A \exp(-\beta_1 |R|) . \quad (9)$$

The adjustable parameters are A and β_1 . $V_{bo}(R_i, R_j)$ is the BO potential, defined as

$$V_{bo}(R_i, R_j) = -B b(R_i, R_j) \exp(-\beta_2 |R_i - R_j|), \quad (10)$$

where $b(R_i, R_j)$ is the "BO function,"

$$b(R_i, R_j) = \chi [1 + \beta^n \zeta_{ij}^n]^{(-1/2n)}, \quad (11)$$

$$\zeta_{ij} = \sum_{k \neq i, j} f_c(|R_i - R_k|) g(\theta_{ijk}), \text{ and} \quad (12)$$

$$g(\theta_{ijk}) = 1 + c \left\{ 1 - 1/[1 + d (h - \cos \theta_{ijk})^2] \right\}. \quad (13)$$

Here, ζ_{ij} is an environmental parameter, and the BO function, $b(R_i, R_j)$, is seen to behave at large ζ as $1/\sqrt{\zeta}$.

In equations 9–13, A , β_1 , B , β_2 , β , χ , n , c , d , and h are the adjustable parameters, and θ_{ijk} is the angle between the bonds i and j and i and k .

The contribution to the energy of the attractive BO potential, V_{bo} , does not have a glue-model form. However, as Brenner (1989) has shown, a Tersoff potential with special parameter values can be reduced to the form of an FS model. The latter is not surprising since the glue-model ideas directly follow from the quantum-mechanical considerations, as does the BO approach.

We will describe a BO potential which basically utilizes the Tersoff ideology but modifies Tersoff's original functions to make the method applicable to transition metals.

3. The Bond-Order Potential for Iron

We preserve the Tersoff's expression for the total energy as

$$E = 1/2 \sum_{i=j} f_c(R_i - R_j) [V_{rep}(R_i - R_j) + V_{bo}(R_i, R_j)]. \quad (14)$$

The repulsion part, $V_{\text{rep}}(R_i - R_j)$, has been modified to allow for a strong repulsion at the distances smaller than half of the nearest neighbor distance in BCC lattice, R_0 , where,

$$V_{\text{rep}}(R) = A \exp \left(-\beta_1 |R| + \beta_4 (0.5R_0/R)^a \right). \quad (15)$$

The attractive, BO part of the energy, is also preserved in

$$V_{\text{bo}}(R_i, R_j) = -B[b(R_i, R_j)] \exp \left(-\beta |R_i - R_j| \right). \quad (16)$$

However, $b(R_i, R_j)$ is now

$$b(R_i, R_j) = \zeta_{ij}^f \left(1 + \gamma_1 \zeta_{ij} + \gamma_2 \zeta_{ij}^2 + \gamma_3 \zeta_{ij}^3 + \gamma_4 \zeta_{ij}^4 + \gamma_5 \zeta_{ij}^5 + \gamma_6 \zeta_{ij}^6 \right), \quad (17)$$

where

$$\zeta_{ij} = \sum_{k \neq i, j} f_c(|R_i - R_k|) g(\theta_{ijk}) \exp \left(-\beta_3 |R_i - R_j|^{\text{nz}} \right). \quad (18)$$

We use the same cut-off function, f_c (equation 10), with the cut-off radii r_{c1} and r_{c2} between the second and third coordination spheres, as in

$$g(\theta_{ijk}) = 1 + c \left\{ 1 - \beta / \left[1 + d(h^2 - \cos \theta_{ijk})^2 \right] \right\}^{2\delta}. \quad (19)$$

Since the Tersoff form of function $b(R_i, R_j)$ was quite arbitrary, with the only requirement of “correct” (reciprocal square root) behavior at large ζ , we decided to try a more general form. The exponent f was allowed to take both positive and negative values.

The adjustable parameters A , β_1 , B , β_2 , β_3 , β , c , d , δ , h , γ_1 , and γ_6^{nz} were found from the following conditions. A and B were found (at fixed values of the other parameters) from two

linear equations for the cohesion energy in BCC modification, E_{coh} at the experimental equilibrium volume Ω_0 , and the pressure $P = 0$ at Ω_0 as shown in Table 1. These equations were solved exactly in an analytical form.

Table 1. Experimental and Fitted Properties of Iron (Energies in eV, Distances in Å, Atomic Volumes in Å³, Elastic Moduli in 10² GPa, and Surface Energy in eV/Surface Atom)

BCC	Exp. Value	Calc. Value
a	2.8589	2.8589
Ω_0	11.6833	11.6833
E_{coh}	-4.28	-4.28
$E_{\text{rep}} = 2.11521; E_{\text{bo}} = -6.3952$		
C11	2.4310	2.3675
C12	1.3810	1.3191
C44	1.2190	1.2190
C'	0.5250	0.5242
K	1.7310	1.6686
$E_{\text{surf}(111)}^a$	2.5	2.2439
FCC($\Omega_0 = 11.152$) ^b		
E_{coh}	-4.223	-4.2229
$(E_{\text{rep}} = 2.4019; E_{\text{bo}} = -6.6249)$		
HCP ($\Omega_0 = 10.398$) ^c		
E_{coh}	-4.213	-4.2134
$(E_{\text{rep}} = 2.9406; E_{\text{bo}} = -7.1540)$		

^a Estimated based on *ab-initio* calculations (Wu and Freeman 1993a, 1993b).

^b The atomic volume and energies as found from experiments on high-temperature BCC-FCC polymorphic transformation (Bendick and Pepperhoff 1982).

^c The atomic volume and energy at the point of BCC-HCP phase transformation (130 kbar) (Giles et al. 1971).

Then, the multivariate minimization procedure (IMSL routine DUMINF) was used. We minimized the root mean square (rms) deviation of the calculated energy from the following Smith-Banerjea universal scaling law (Banerjea and Smith 1988):

$$E_{us} = E_{coh} (1 + s) \exp(-s), \quad (20)$$

where

$$s = 4.85406479 (-E_{coh}/k \cdot s_0). \quad (21)$$

K is the bulk modulus (in Mbar), and s_0 is the Wigner-Seitz radius (in Å), which corresponds to the equilibrium atomic volume Ω_0 .

Other conditions to be imposed on the adjustable parameters were:

- The calculated elastic moduli, C' , and C_{44} had to be as close as possible to their experimental values in BCC lattice. The bulk modulus, K , would be automatically close to its experimental value if the rms universal scaling minimization had been achieved.
- The calculated energies of FCC and HCP modifications at the corresponding volumes had to be as close as possible to the corresponding experimental energies for FCC and HCP lattices.
- The calculated (111) free surface energy for BCC lattice had to be as close as possible to the corresponding experimental or *ab-initio* value.

These three conditions were fulfilled by making use of five punishment functions equal to one if the experimental and calculated quantities to be fitted were exactly equal; the function would otherwise be growing as a factor times the corresponding quadratic deviation. By changing the values assigned to the factors, the minimization process could be directed towards damping down the undesirable deviation.

Parameter nz , which enters the expression for the total energy, was set by trial-and-error tests $nz = 6$. We “switched off” the short range repulsion, $\beta_4 = 0$. In the future, a more appropriate

choice of the value for β_4 will be accepted; however, a strong increase of the short-range repulsion will hardly affect the energy at physically reasonable distances but may be important in molecular dynamics-type atomistic simulations to prevent nonphysical configurations from occurring.

Tables 1 and 2 present the results of the parameter optimization. Table 1 shows that the new potential reproduces the elastic moduli with very high precision. It is well known that C_{44} is

Table 2. Parameters of the Potential

$V_{\text{rep}} = A \exp (-\beta_1 R + \beta_4 (R/0.5R_0)^\alpha)$
$A = 0.2346154E + 04$
$\beta_1 = 0.3465077E + 01$
$\beta_4 = 0$
$\alpha = 0$
$V_{\text{bo}}(R_i, R_j) = B b(R_i, R_j) \exp [(-\beta_2 R_{ij}]$
$B = 0.1580257E - 04$
$\beta_2 = 0.1117197E + 01$
$b = \zeta^f(1 + \gamma_1\zeta + \dots \gamma_6\zeta^6)$
$f = 0.4534376E + 00$
$\gamma_1 = 0.3718635E + 03$
$\gamma_2 = 0.1664427E + 04$
$\gamma_3 = -0.6539821E + 02$
$\gamma_4 = 0.9013512E + 00$
$\gamma_5 = -0.1142012E - 01$
$\gamma_6 = 0.1385744E - 03$
$\zeta = \sum f_c(R_{ik} g(\theta_{ijk}) \exp [(\beta_3 R_{ik} ^{nz}]$
f_c (equation 5): Cut-off radii:
$r_{c1} = 3.70, r_{c2} = 3.60$
$nz = 6, \beta_3 = 0.6034363E + 00$
$g = 1 + c \{1 - \beta/[1 + d (h^2 - \cos\theta^2)^2]\}^{(2\delta)}$
$\beta = 0.9433671E + 00$
$\delta = 0.9870393E + 00$
$c = 0.419903E + 01$
$d = 0.3752465E + 02$
$h = 0.6915982E + 00$

especially sensitive to directional bonding and is not reproduced well by the traditional EAM. The energies of FCC and HCP are also well reproduced.

An interesting feature of the potential is that the exponent f in the BO function is very close to 0.5 (0.4534376), rather than -0.5 . In order to correctly reproduce the energies of FCC and HCP modifications, the BO function has to increase with ζ rather than decrease. Our attempts to modify the function so that it behaved correctly at large ζ failed.

Figures 1–3 illustrate some of the results of the parameter fitting. Figure 1 shows the total energy as a function of the volume ratio $\Omega/\Omega_0^{\text{BCC}}$, (Ω_0^{BCC} is the atomic volume of BCC iron at equilibrium) as compared to the universal scaling curve, equation 14. Figure 2 compares the calculated volume-pressure equation of state $\Omega/\Omega_0^{\text{BCC}}(P)$ with experimental data; the agreement is excellent.

Fitting the energies of FCC and HCP phases of iron was part of the procedure of the potential calibration. The HCP experimental energy was estimated from the enthalpy at the point of BCC-HCP phase transformation under pressure at 130 kbar. Figure 3 shows the enthalpies (H) of BCC and HCP phases as functions of pressure. One can see that the phase transformation occurs at $P = 110$ kbar. This should be considered as a reasonable agreement with the experimental value of 130 kbar.

4. Conclusion

We have developed a semi-empirical BO potential for iron, and the preliminary results look encouraging. Although some further testing and possibly further readjustment of the potential parameters may be needed, hopefully the new potential will be instrumental in atomistic simulations of both deformation processes in iron and chemisorption reactions on iron surfaces.

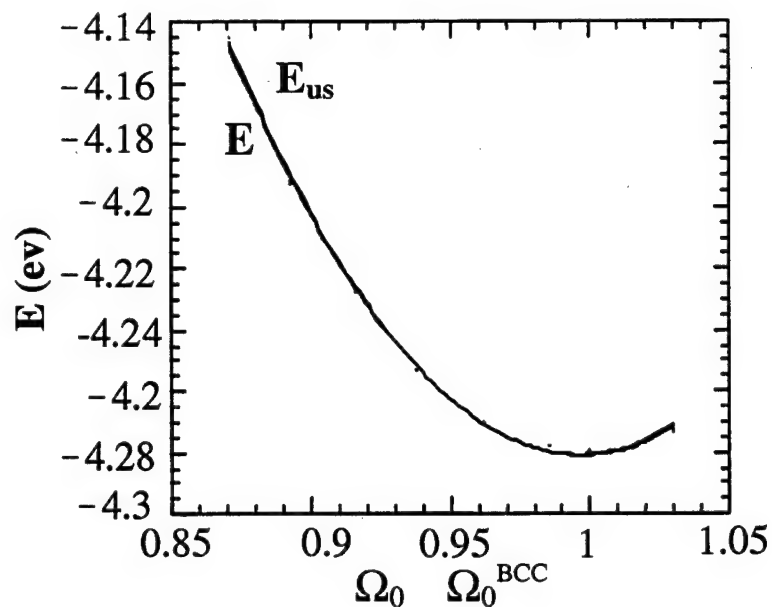
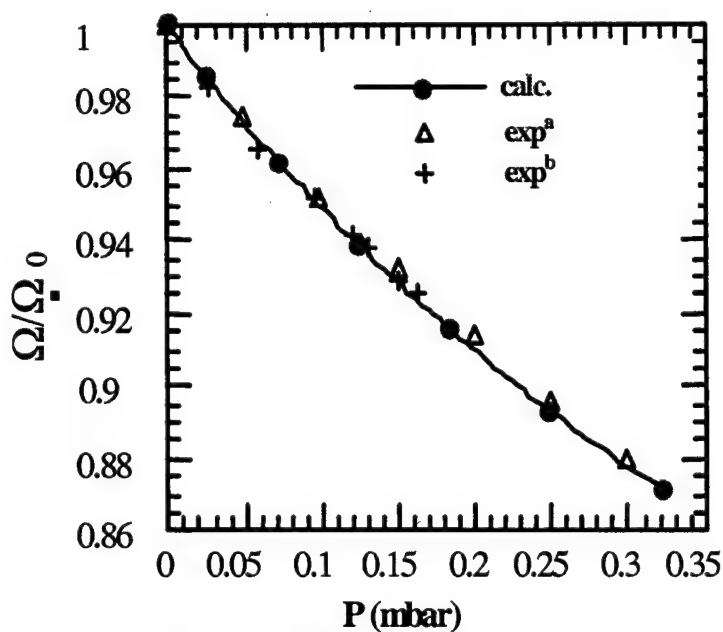


Figure 1. Comparison of the Calculated Volume Dependence of the Cohesive Energy With the Universal Scaling (E_{us}) Curve (Banerjee and Smith 1998).



^a Giles et al. 1971.

^b Clendener and Drickamer 1964.

Figure 2. The Calculated Equation of States for BCC Iron.

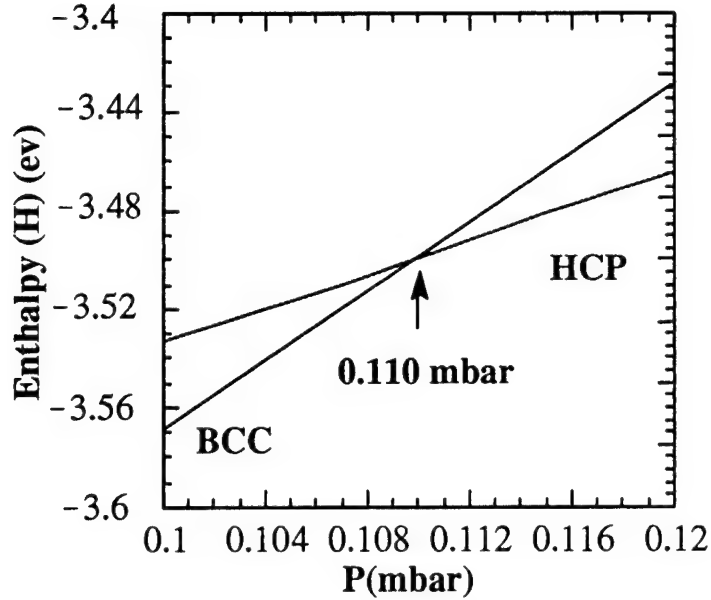


Figure 3. The BCC-HCP Phase Transformation Under Pressure.

Recently, a method of explicitly calculating ferromagnetic contributions to the total energy in iron based on the Stoner model of itinerant ferromagnetism was suggested (Krasko 1996; Shibutani et al., to be published). If successful, this method may become an ultimate tool for atomistic simulations in iron. While the detailed implementation and testing of this method are still in the future, the new BO potential will enable valuable information on some important processes in iron to be obtained. A BO potential of the same type will also be used in the Stoner model method for evaluating the nonmagnetic contributions to the total energy.

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